

The Effect of Reservoir Temperature and Applied Pore Pressure on the Pore-Scale Imbibition in Shales

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GEOProc 2015, February 26, 2015
Salt Lake City, Utah, United States

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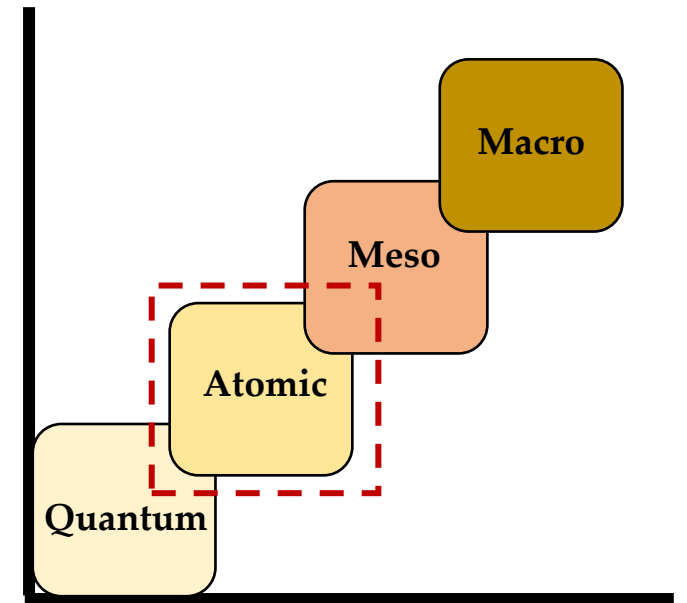


Overview

- Research background
- Development of an atomistic pore model
- Molecular dynamics simulation details
- Results and discussion
- Conclusion

Research background

- A pore-scale multiphase transport is **poorly understood** in unconventional reservoirs due to:
 - ❑ Heterogeneous nature of the reservoir
 - ❑ Highly complex multiscale pore structure
 - ❑ Ultralow permeability
 - ❑ Limitations of core-flooding experiments and numerical models to provide an in-depth comprehension of the pore-scale processes
- A multiscale reservoir simulation is necessary
- The molecular dynamics (MD) approach is a potential simulation tool to model a pore-scale fluid transport and enhance our present fundamental understanding of fluid flow in unconventional reservoirs



Development of an atomistic pore-scale model (1)

- Realistic pore description is necessary to develop a three-dimensional atomistic pore model
- A workflow is proposed to fulfil this objective and shown in Fig. 1

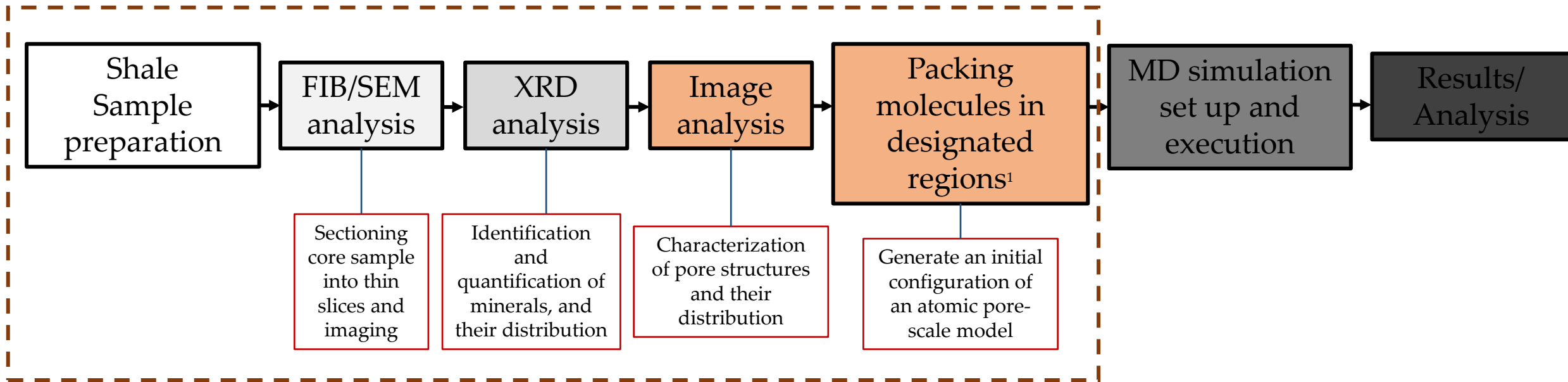


Figure 1: Workflow to develop an atomistic pore-scale model

Development of an atomistic pore-scale model (2)

- Figure shows an atomistic pore-scale model replicating shale matrix
- 5 nm pore is considered in present study

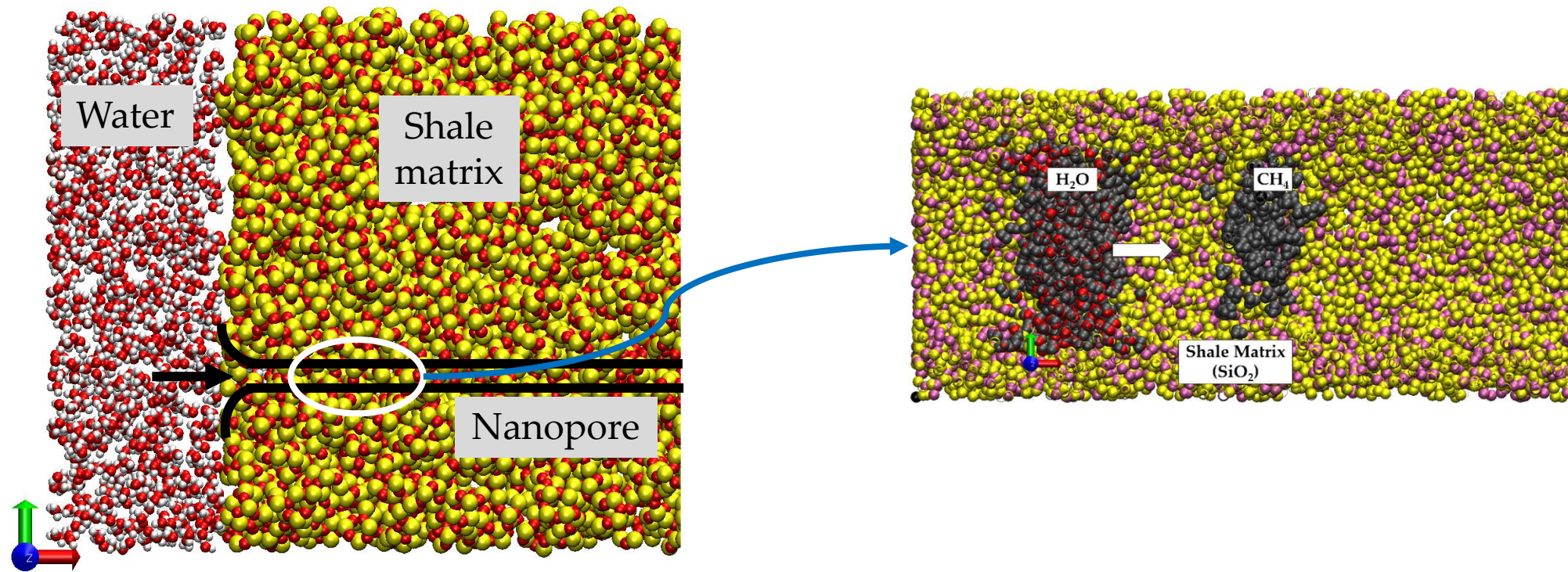


Figure 2: Atomistic pore model of 5 nm shale nanopore

Molecular dynamics simulation workflow

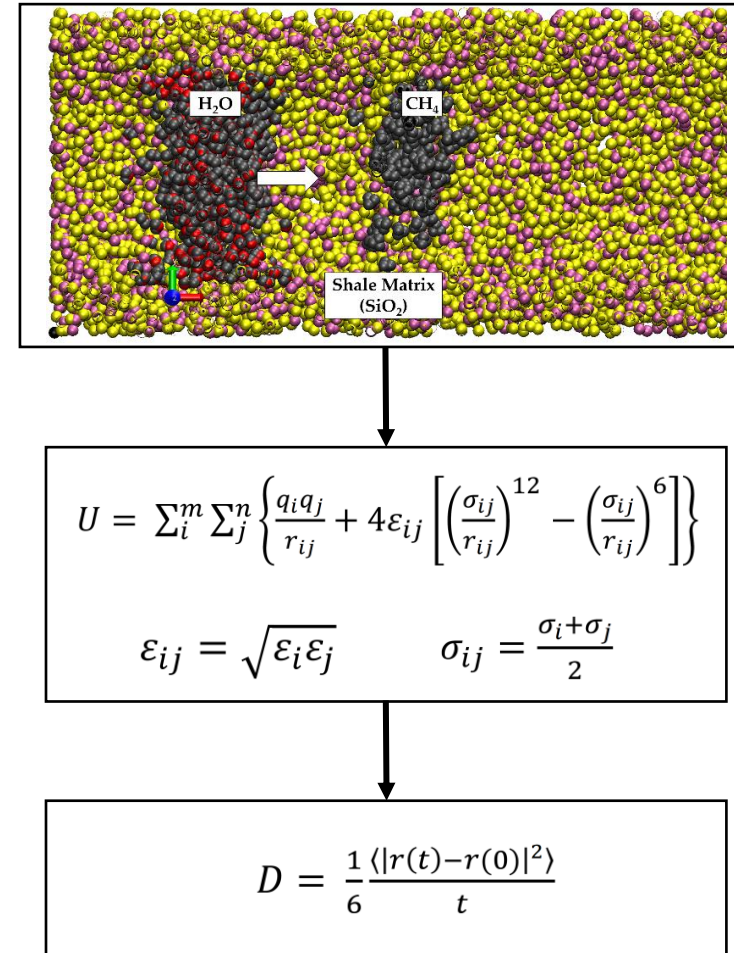
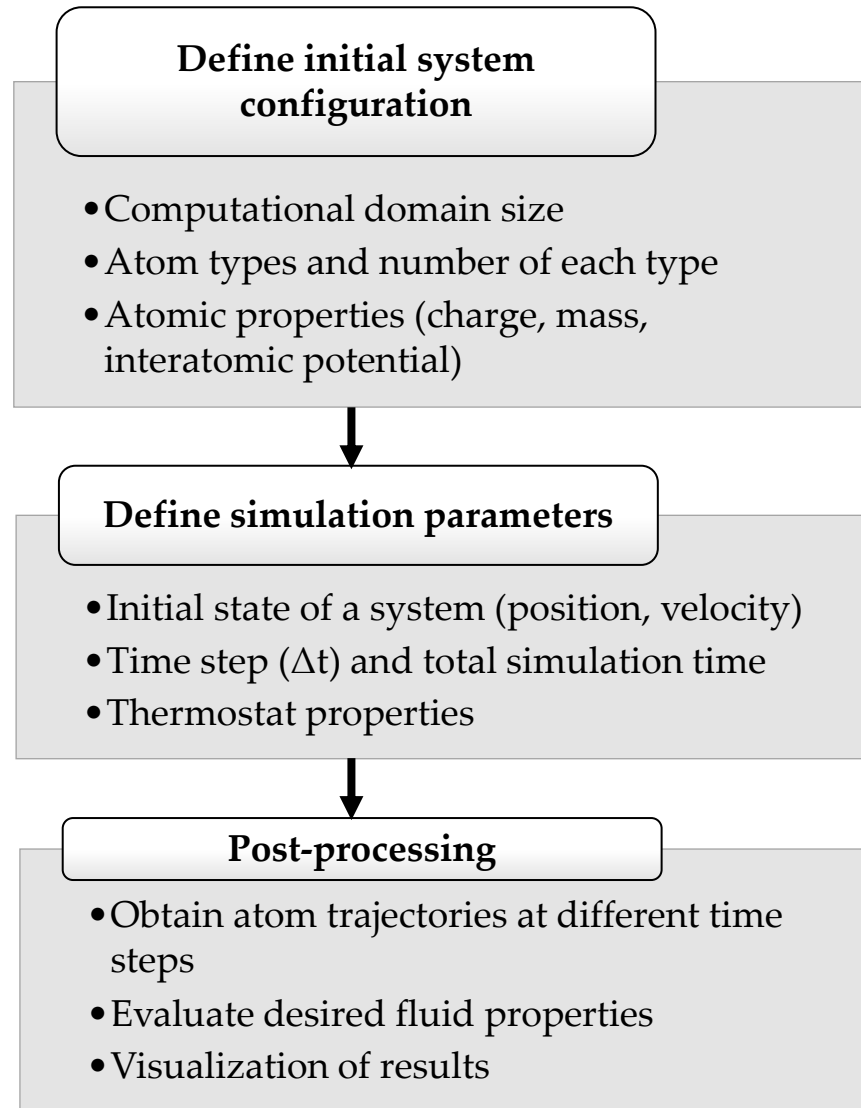
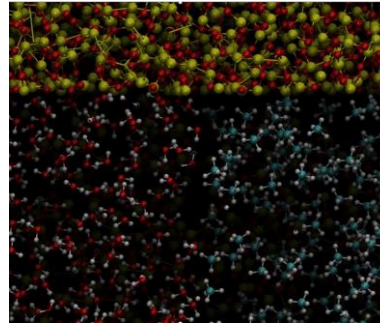
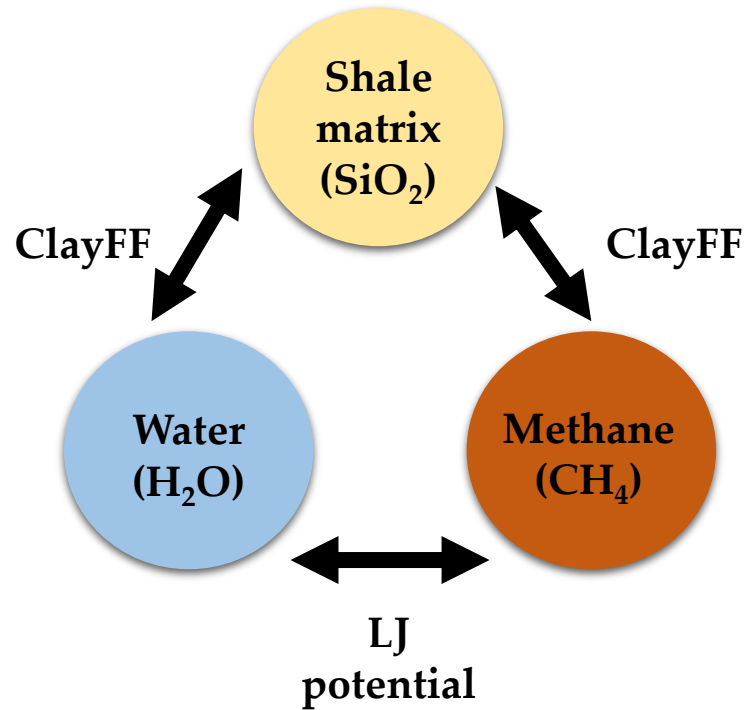
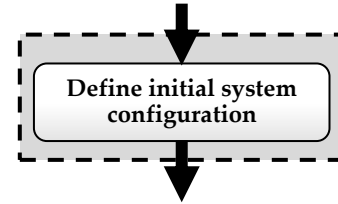


Figure 3: Molecular dynamics workflow

Interatomic potential parameters

- Table 1 summarizes the force field and interatomic potential parameters
- Lorentz-Berthelot rule is used to evaluate properties for the dissimilar atoms



Parameter	ϵ [kJ/mol]	σ [Å]	q [e ⁻]
O (water)	0.6502	3.166	-0.8476
H (water)	-	-	0.4238
C (methane)	1.231	3.73	-
Si (quartz)	0.5335	3.795	2.4
O (quartz)	0.6487	3.154	-1.2

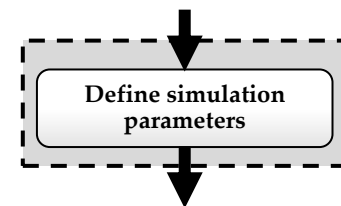
Figure 4: Force field representation

Table 1: Interatomic potential force field and parameters^{2, 3, 4, 5}

Additional MD Simulation Details

- LAMMPS⁶ used to perform MD simulations

Parameter	Value
Number of water molecules	1285
Number of methane molecules	191
Number of quartz unit cells	5337
Total simulation time	40,000 fs with 0.01 fs time-step
Applied force on water molecules	0, 5 and 10 Kcal/mol-Å
System temperature	350 °K



- Temporal atomic positions obtained to calculate important transport properties including
 - ☐ Mean square displacements,
 - ☐ Self-diffusion coefficients,
 - ☐ Relative mobility ratio between molecules

Results and discussion (1): Temporal positions

- Figure 5 shows the temporal advancement (imbibition) of water and methane molecules in methane saturated shale nanopore with 5 nm diameter
- At 0 Kcal/mol-Å (self-diffusion of molecules) methane recovery rate is extremely slow whereas the recovery rate increases with an increase in applied force on water molecules

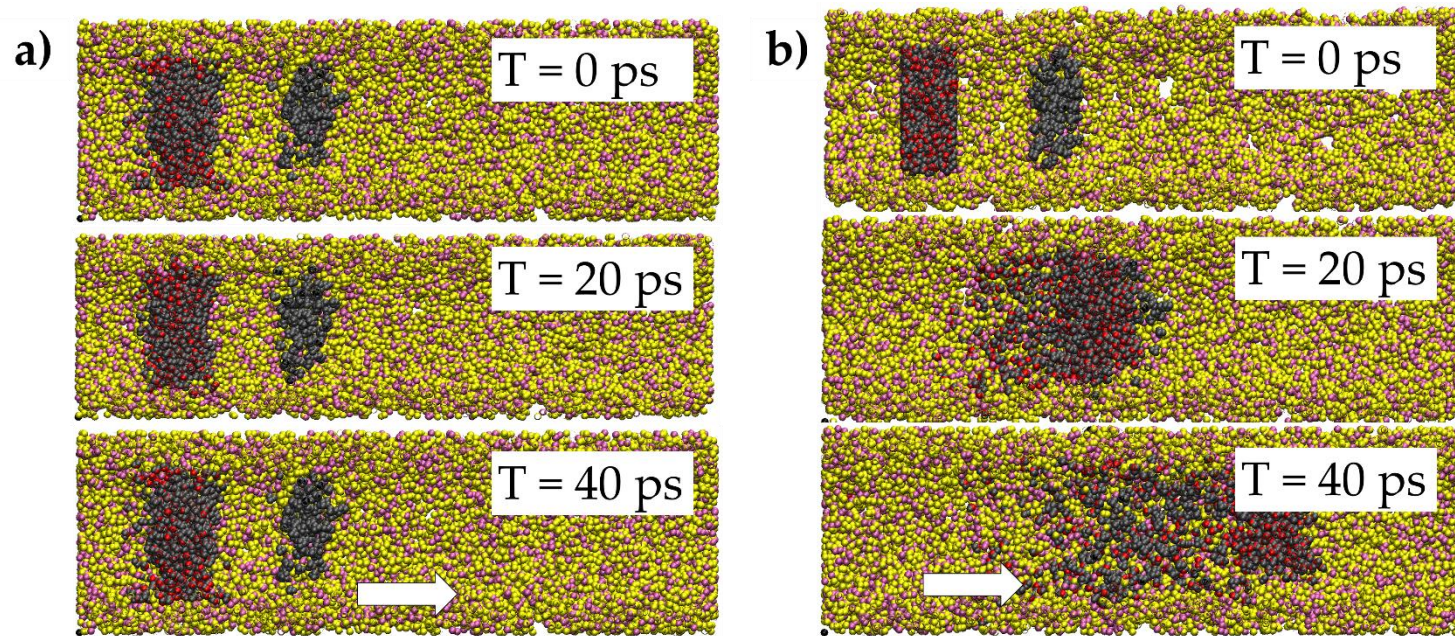
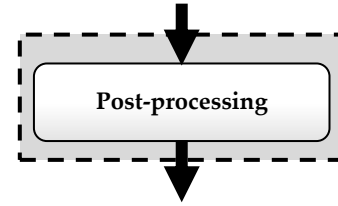
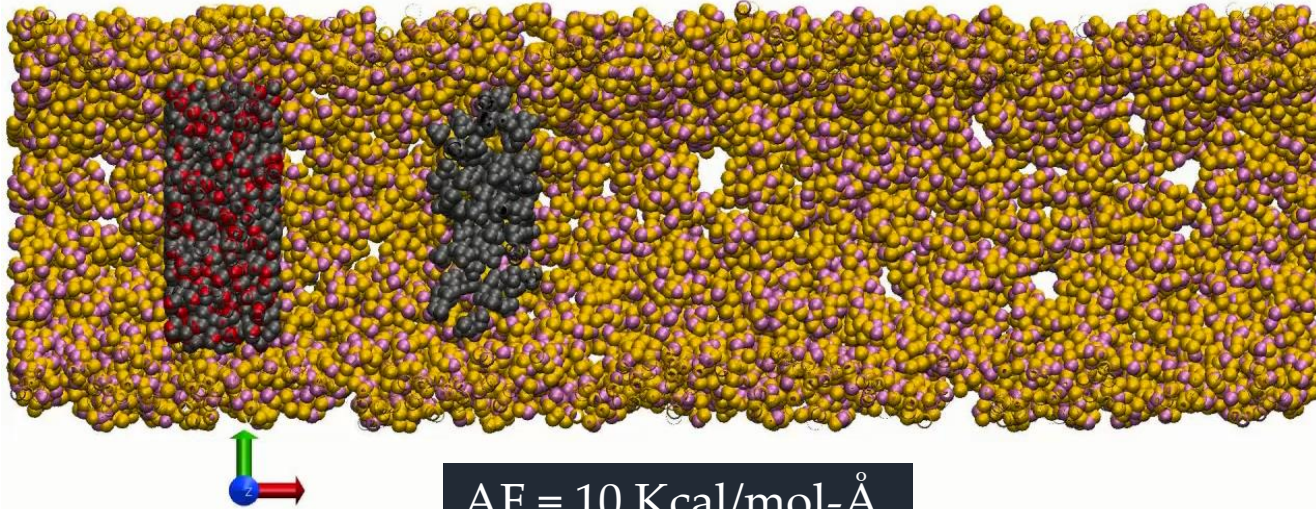


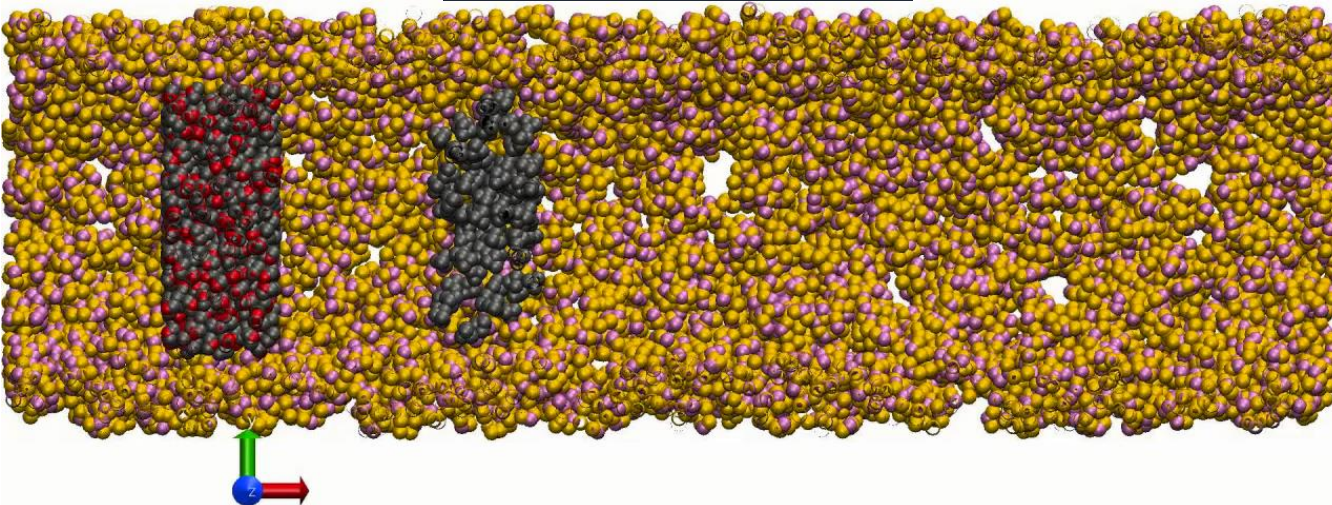
Figure 5: Multiphase fluid imbibition in a shale nanopore for applied force of a) 0 Kcal/mol-Å b) 10 Kcal/mol-Å

Results and discussion (2): Temporal positions

$AF = 0 \text{ Kcal/mol-Å}$



$AF = 10 \text{ Kcal/mol-Å}$



- Self-diffusion of molecules
- Extremely slow recovery process

- Improved recovery rates
- Adsorption of molecules in shale matrix

Results and discussion (3): MSD for water

- Mean square displacement of water (MSD_w) is evaluated for 40,000 fs
- MSD_w increases with an increase in time and applied pore pressure
- Self-diffusion coefficient is evaluated (force of 0 Kcal/mol-Å) and found to be $0.4939 \times 10^{-9} \text{ m}^2/\text{s}$

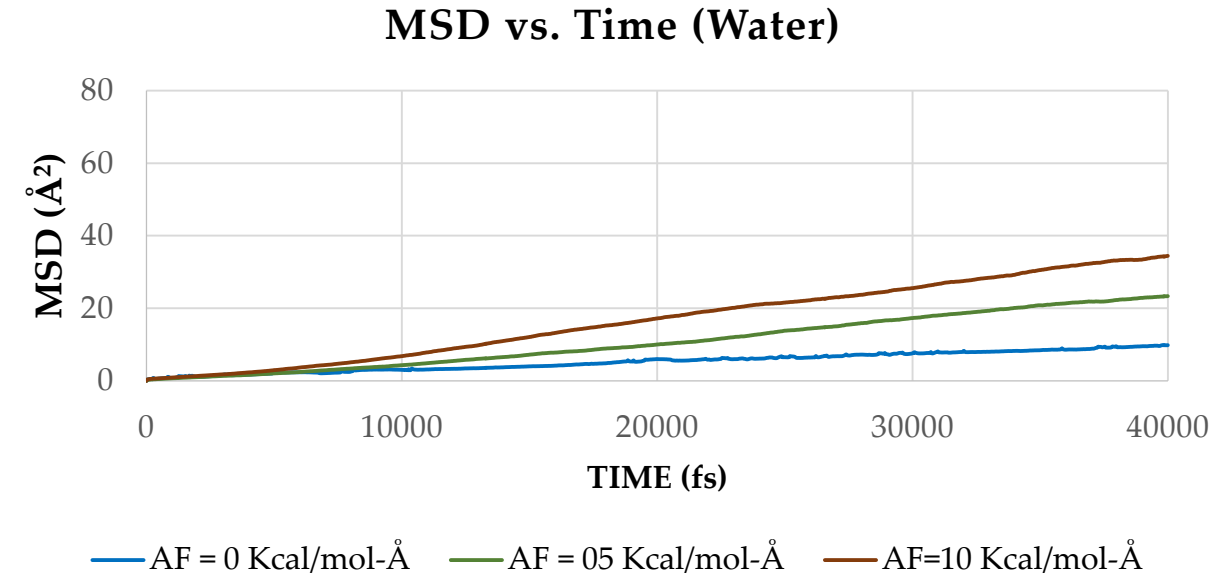


Figure 6: Mean square displacement of water

Results and discussion (4): MSD for Methane

- Mean square displacement of methane (MSD_m) is evaluated for 40,000 fs
- Similar trend in MSD_m is observed for time and applied water force
- Comparatively higher values of MSD_m observed for methane than water for an increased applied pore pressure
- Self-diffusion coefficient of methane is evaluated and found to be $0.3514 \times 10^{-9} \text{ m}^2/\text{s}$

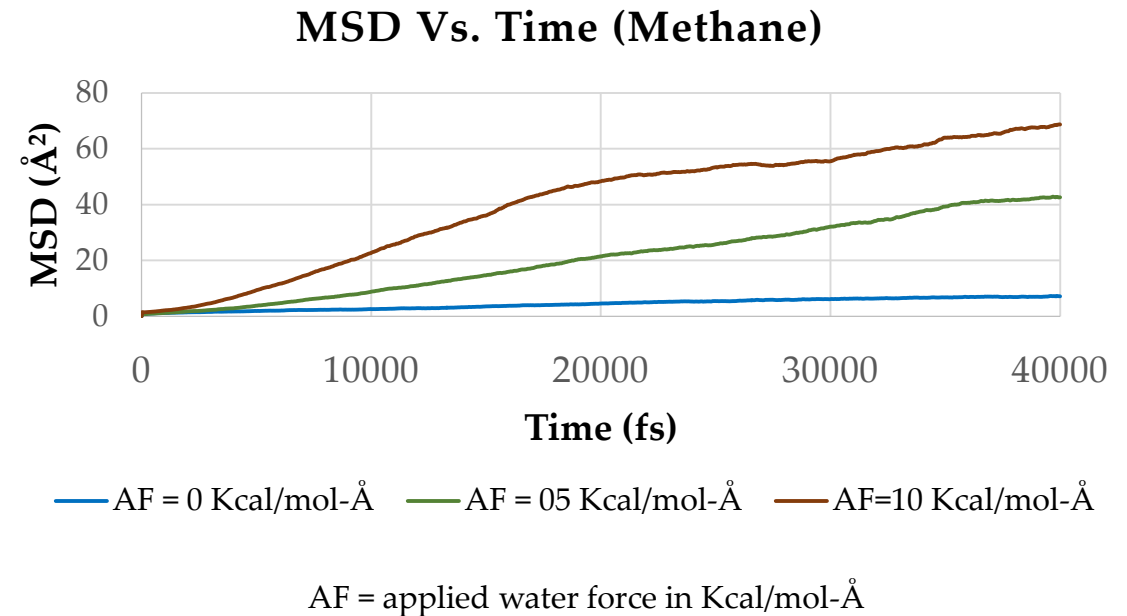


Figure 7: Mean square displacement of methane

Results and discussion (5) : Relative mobility ratio

- RMR is defined as the ratio of MSD_m and MSD_w
- RMR provides a comparative displacement between methane and water
- Higher RMR values are favorable as they represents **higher mobility** thus **higher recovery** rate of methane
- Rate of RMR is increases rapidly initially (equilibration of system) and then stabilizes

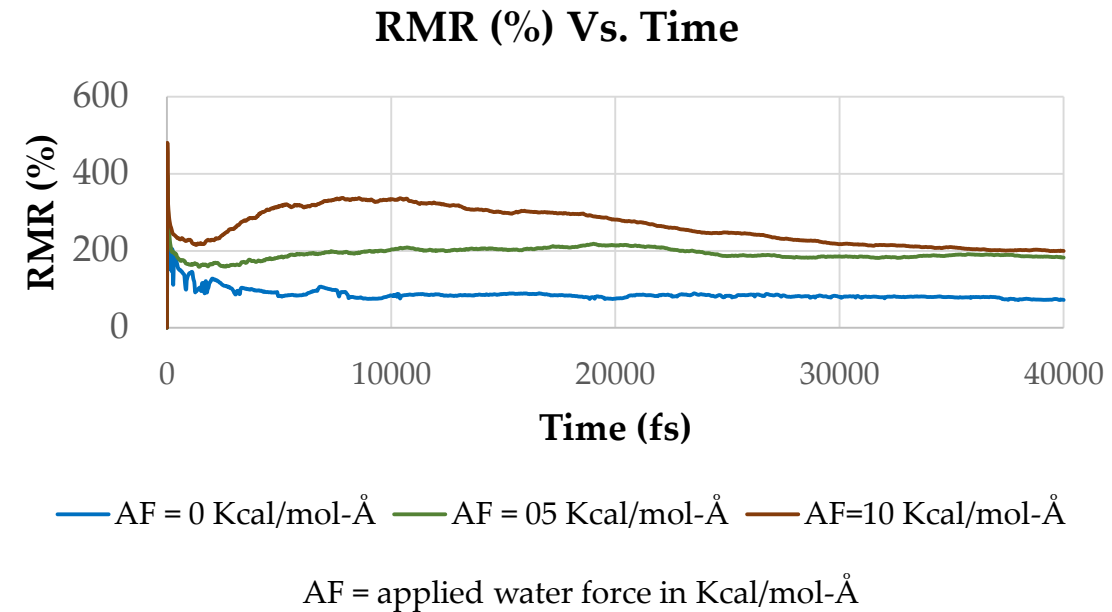


Figure 8: Relative mobility ratio between methane and water

Results and discussion (6): Computational time analysis

- Typical MD simulation time distribution is shown in Fig. 9a
- Kspace calculations are the most computationally expensive in MD
- Computational performance compared for 5000 steps with 0.001 fs time step
- The total computational time decreases with an increase in the number of processors
- No major difference observed in total simulation time for various applied forces

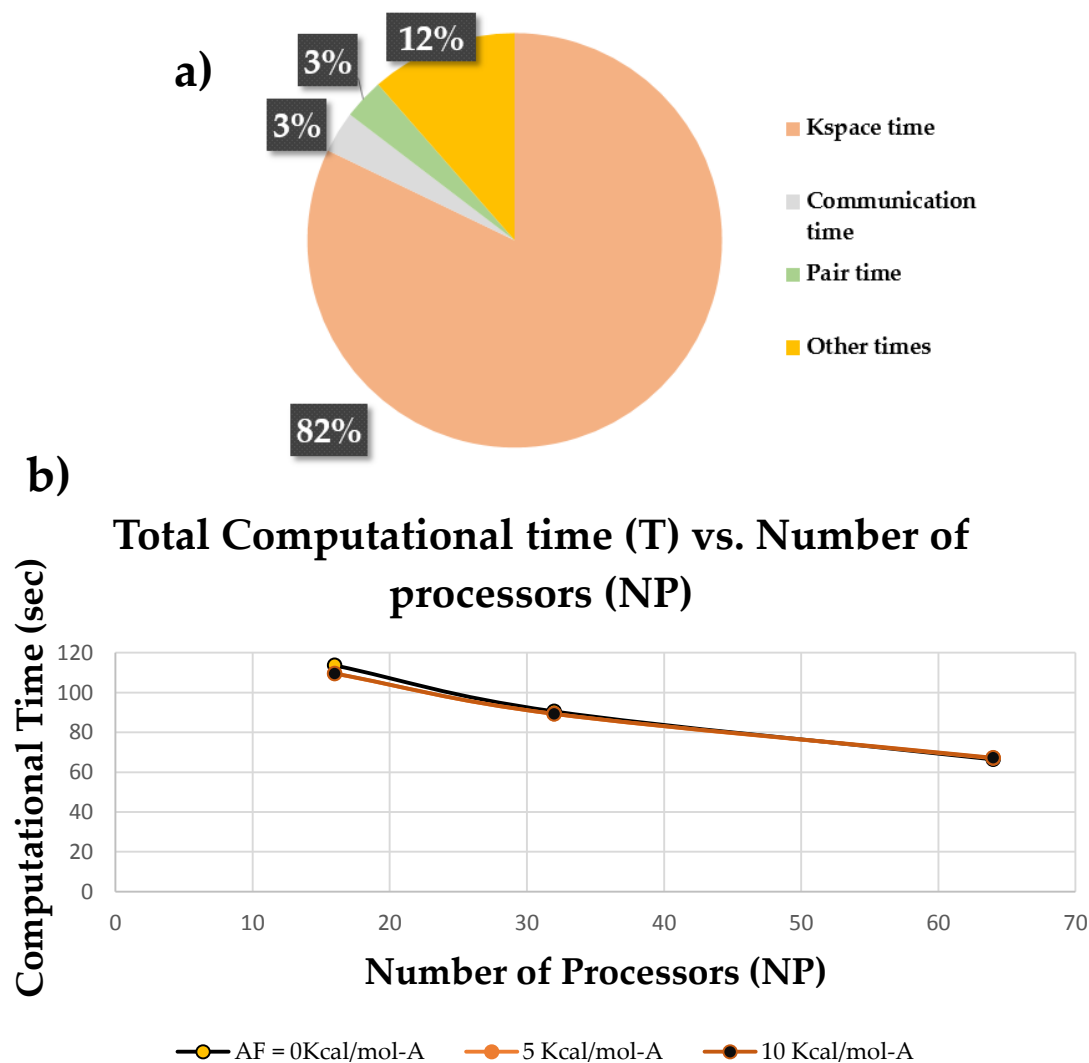


Figure 9: Computational performance

Conclusion

- A molecular dynamics approach is presented for the **pore-scale transport modeling**
- Thorough insight of transport process at atomic level in shale nanopores can be obtained
- Hydrocarbon recovery can be expected from shale nanopores provided higher pressure differential exists in pores
- The molecular simulation method can be extended to address challenges in enhanced oil and gas recovery by modeling
 - ❑ Pore-scale shale oil recovery
 - ❑ Pore swelling
 - ❑ Hydraulic fracturing
 - ❑ Carbon sequestration

Acknowledgement

We would like to thank the Center for High Performance Computing (CHPC), University of Utah for the access to parallel computing.

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THANK YOU